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PHYSICS-PRESERVING TURBULENT CLOSURE MODELS

SGS Flux Vectors of Mass and Energy

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Abstract. Both necessary and sufficient conditions are derived in a systematic, rigorous way for a subgrid-scale (SGS) flux vector model to preserve the frame-indifference of the vector and to satisfy both the principle of material frame indifference (PMFI) and the second law of thermodynamics. This leads to the results either confirming the previous intuitive arguments or offering new insights into turbulence modelling, and is of significance in clarifying some controversies in the literature, examining how well existing models preserve the physics, and developing new models.

1. Introduction

SGS stresses and fluxes of mass and energy are believed to be quantities determined by filtered large-scale velocity and mass fraction/temperature fields in the large eddy simulation (LES). Based on this fundamental, intrinsic belief, various approaches have been proposed to relate SGS stresses and fluxes to the filtered large-scale fields, so-called SGS turbulence modelling. The readers are referred to Ciofalo (1994), Mason (1994), Lesieur & Métais (1996) and Sagaut (2001) for some recent excellent reviews and discussions of this important topic. While some LES results based on some commonly used models seem encouraging, they fail to meet either one or both of two natural fundamental requirements for turbulence models: preserving the fundamental properties of the quantities being modeled and satisfying some classical principles.

The modelling of the SGS flux vectors of mass and energy consists of replacing them by constitutive equations expressing them as functions of filtered large-scale fields of velocity and mass fraction/temperature. While such constitutive equations may take different forms such as algebraic and differential, it appears to be a basic requirement to preserve the properties

which the flux vectors hold by their definition. Such a property is the frame-indifference (Fureby & Tabor 1997, Ghosal 1999, Wang 2001). It follows from the definition of the SGS flux vectors and states that they remain the same directed line element under a change of frame. The issue concerned with whether a model guarantees this property is referred as the invariance in the literature.

While the first requirement focuses on the properties of the SGS flux vectors themselves, the second requirement emphases on their *function relation* with the filtered large-scale fields. Such function relations are required to satisfy some classical principles including the PMFI and the second law of thermodynamics (Fureby & Tabor 1997, Ghosal 1999, Wang 1997, 1999, 2001). The PMFI requires that the function relation is the same for every observer, i.e. in every frame of reference. The second law of thermodynamics, on the other hand, states that the flux is always from high concentration to low concentration. Note that the realizability for the Reynolds and SGS stresses also comes from the second law of thermodynamics (Wang 1999, 2001).

The motivation for the present work comes from the desire to derive *both* necessary and sufficient condition in a systematic, rigorous way for a SGS flux model to preserve the frame-indifference of SGS flux vectors and to satisfy both the PMFI and the second law of thermodynamics. Unlike the works in the literature, no intuitive assumption is introduced in the derivation; the independent variables are chosen properly; the PMFI and the frame indifference of SGS flux vectors are clearly distinguished. This leads to some conclusive results. Among them, some confirm the previous intuitive arguments, and others form new insights to SGS turbulence modelling.

2. Principle of Material Frame-Indifference and Second Law of Thermodynamics

Consider a class of constitutive relations which relate the passive SGS flux vector $\mathbf{q}$ of mass or energy to its arguments $\theta, O.P., \nabla\theta, \mathbf{v}, \mathbf{L}$, i.e.,

$$\mathbf{q} = \mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{v}, \mathbf{L}). \tag{1}$$

Here $\mathbf{f}$ is a vector-valued function. θ is the concentration of a property. It is the mass fraction of a species for the case of SGS flux of mass, and the temperature when $\mathbf{q}$ is the SGS flux of energy. $O.P.$ denotes the other scalar-valued thermophysical parameters which are independent of $\mathbf{v}$ and $\mathbf{L}$ and are typically the local thermodynamic state variables. $\nabla\theta$ is the gradient of θ. $\mathbf{v}$ is the filtered velocity vector. $\mathbf{L}$ is the velocity gradient tensor of $\mathbf{v}$, a second order tensor-valued variable.

In sharp contrast with that in the literature, we choose $\mathbf{L}$ as an independent variable instead of its symmetric part $\mathbf{D}$ (the velocity strain tensor) and skew part $\mathbf{W}$ (the vorticity tensor) because $\mathbf{D}$ and $\mathbf{W}$ can not be regarded as independent. We do not include k, l or ε as the independent variables. The exclusion of the explicit dependence of $\mathbf{q}$ on time t and position vector $\mathbf{r}$ comes from the fact that they affect $\mathbf{q}$ through θ, $O.P.$, $\nabla\theta$, $\mathbf{v}$ and $\mathbf{L}$.

The relation (1) satisfies both principle of determinism and principle of local action since we assume that $\mathbf{q}$ at a point and a time instant is a function of its arguments at that point and that instant.

The principle of frame-indifference requires that $\mathbf{f}$ is the same for every observer, i.e.

$$\mathbf{q}^* = \mathbf{f}(\theta^*, O.P.^*, (\nabla\theta^*)^*, \mathbf{v}^*, \mathbf{L}^*) \tag{2}$$

in which superscript $*$ represents the quantities observed by another observer $*$.

The second law of thermodynamics states that $\mathbf{q}$ is always from high concentration to low concentration. This requires that: (1) $\mathbf{f}$ changes its sign if $\nabla\theta$ changes the sign, i.e.,

$$\mathbf{f}(\theta, O.P., -\nabla\theta, \mathbf{v}, \mathbf{L}) = -\mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{v}, \mathbf{L}), \tag{3}$$

and (2) the projection of the $\mathbf{f}$ on $\nabla\theta$ is negative semi-definite, i.e.,

$$\mathbf{f} \cdot \nabla\theta \le 0. \tag{4}$$

2.1. NECESSARY CONDITIONS FOR REQUIREMENTS (2) AND (3)

2.1.1. $\mathbf{q} - \mathbf{v}$ *relation*

Theorem 1. $\mathbf{f}$ *is independent of* $\mathbf{v}$.

Proof From the principle of observer transformations (Geankoplis 1983, Truesdell 1991),

$$\left.\begin{array}{lll} \theta^* = \theta, & (O.P.)^* = O.P., & \mathbf{q}^* = \mathbf{Q}(t)\mathbf{q}, \\ (\nabla\theta^*)^* = \mathbf{Q}(t)\nabla\theta, & \mathbf{L}^* = \mathbf{Q}(t)\mathbf{L}\mathbf{Q}^T(t) + \dot{\mathbf{Q}}(t)\mathbf{Q}^T(t), & \\ \mathbf{r}^* = \mathbf{Q}(t)\mathbf{r} + \mathbf{c}(t), & \mathbf{v}^* = \frac{dr^*}{dt} = \dot{\mathbf{Q}}(t)\mathbf{r} + \mathbf{Q}(t)\mathbf{v} + \dot{\mathbf{c}}(t), & \end{array}\right\} \tag{5}$$

where $\mathbf{Q}$ is an arbitrary rotation tensor, $\mathbf{r}$ a position vector of material point, $\mathbf{c}(t)$ an arbitrary vector-valued function of time t, and a dot over a letter indicates a time derivative. In (5), we have used the frame indifference of $\mathbf{q}$.

By making use of (1) and (5), (2) yields (suppressing t)

$$\mathbf{f}(\theta, O.P., \mathbf{Q}\nabla\theta, \dot{\mathbf{Q}}\mathbf{r} + \mathbf{Q}\mathbf{v} + \dot{\mathbf{c}}, \mathbf{Q}\mathbf{L}\mathbf{Q}^T + \dot{\mathbf{Q}}\mathbf{Q}^T) = \mathbf{Q}\mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{v}, \mathbf{L}),$$
$$\forall \mathbf{Q} \text{ and } \mathbf{c}. \tag{6}$$

Since (6) holds for all $\mathbf{Q}$, it must be true for $\mathbf{Q} = \mathbf{1}$. Take $\mathbf{Q} = \mathbf{1}$, then $\dot{\mathbf{Q}} = \mathbf{0}$. Equation (6) reduces to

$$\mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{v} + \dot{\mathbf{c}}, \mathbf{L}) = \mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{v}, \mathbf{L}) \quad \forall \dot{\mathbf{c}}. \tag{7}$$

This implies that $\mathbf{f}$ is independent of velocity $\mathbf{v}$.

By applying Theorem 1, (1) and (6) reduce to

$$\mathbf{q} = \mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{L}), \tag{8}$$

$$\mathbf{f}(\theta, O.P., \mathbf{Q}\nabla\theta, \mathbf{Q}\mathbf{L}\mathbf{Q}^T + \dot{\mathbf{Q}}\mathbf{Q}^T) = \mathbf{Q}\mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{L}) \quad \forall \mathbf{Q}. \tag{9}$$

2.1.2. $\mathbf{q} - \mathbf{L}$ *relation*

Note that $\mathbf{L}$ can be uniquely decomposed into a symmetric tensor $\mathbf{D}$ (velocity strain tensor) and a skew tensor $\mathbf{W}$ (vorticity tensor). Expression (9) may, then, be rewritten as

$$\mathbf{f}(\theta, O.P., \mathbf{Q}\nabla\theta, \mathbf{Q}\mathbf{D}\mathbf{Q}^T + \mathbf{Q}\mathbf{W}\mathbf{Q}^T + \dot{\mathbf{Q}}\mathbf{Q}^T) = \mathbf{Q}\mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{L}) \quad \forall \mathbf{Q}. \tag{10}$$

Theorem 2. *For rotation tensor $\mathbf{Q}(t) = exp[\hat{\mathbf{\Omega}}(t - \tau)]\hat{\mathbf{Q}}$, we can, at any instant τ, pick $\mathbf{Q}(\tau)$ and $\mathbf{Q}(\tau)\mathbf{Q}^T(\tau)$ to be arbitrary, independent rotation and skew tensors, respectively. Here $\hat{\mathbf{Q}}$ is any time-independent rotation tensor, and $\hat{\mathbf{\Omega}}$ any time-independent skew tensor.*

Proof As $\hat{\mathbf{\Omega}}$ is a time-independent skew tensor, $exp[\hat{\mathbf{\Omega}}(t - \tau)]$ is thus a rotation tensor for any fixed time τ and all time t. Since both $\hat{\mathbf{Q}}$ and $exp[\hat{\mathbf{\Omega}}(t - \tau)]$ are rotation tensors, $\mathbf{Q}(t) = exp[\hat{\mathbf{\Omega}}(t - \tau)]\hat{\mathbf{Q}}$ is also a rotation tensor for all time t. Also,

$$\mathbf{Q}(\tau) = \hat{\mathbf{Q}}, \tag{11}$$

$$\dot{\mathbf{Q}}(\tau)\mathbf{Q}^T(\tau) = \hat{\mathbf{\Omega}}\mathbf{Q}(\tau)\mathbf{Q}^T(\tau) = \hat{\mathbf{\Omega}}. \tag{12}$$

They are clearly independent rotation and skew tensors if $\hat{\mathbf{Q}}$ and $\hat{\mathbf{\Omega}}$ are any time-independent rotation and skew tensors, respectively.

Theorem 3. $\mathbf{L}$ *affects* $\mathbf{q}$ *only through velocity strain tensor* $\mathbf{D}$.

Proof To prove this, choose $\mathbf{Q}(t)$ defined in Theorem 2 as the rotation tensor in (10) while for any instant τ, $-\mathbf{Q}\mathbf{W}\mathbf{Q}^T \mid_\tau$ is used as the skew

tensor $\hat{\mathbf{\Omega}}$, i.e. $\hat{\mathbf{\Omega}} = -\mathbf{Q}\mathbf{W}\mathbf{Q}^T \mid_\tau$ (Such a $\hat{\mathbf{\Omega}}$ do a skew tensor since $\hat{\mathbf{\Omega}}^T = -\mathbf{Q}\mathbf{W}^T\mathbf{Q}^T \mid_\tau = \mathbf{Q}\mathbf{W}\mathbf{Q}^T \mid_\tau = -\hat{\mathbf{\Omega}}$). Then at time $t = \tau$, (10) yields

$$\mathbf{f}(\theta, O.P., \hat{\mathbf{Q}}\nabla\theta, \hat{\mathbf{Q}}\mathbf{D}\hat{\mathbf{Q}}^T) = \hat{\mathbf{Q}}\mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{L}) \quad \forall\hat{\mathbf{Q}}. \tag{13}$$

As this is true for all rotation tensor $\hat{\mathbf{Q}}$, it must hold for $\hat{\mathbf{Q}} = \mathbf{1}$. Let $\hat{\mathbf{Q}} = \mathbf{1}$, (13) yields

$$\mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{L}) = \mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{D}), \tag{14}$$

or

$$\mathbf{q} = \mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{D}). \tag{15}$$

2.1.3. $\mathbf{q}$-$\nabla\theta$ *relation*

Expression (15) and the principle of frame-indifference together yield

$$\mathbf{q}^* = \mathbf{f}(\theta^*, (O.P.)^*, (\nabla\theta^*)^*, \mathbf{D}^*) \tag{16}$$

By making use of (5), (15) and $\mathbf{D}^* = \mathbf{Q}\mathbf{D}\mathbf{Q}^T$ (Truesdell 1991), (16) leads to

$$\mathbf{f}(\theta, O.P., \mathbf{Q}\nabla\theta, \mathbf{Q}\mathbf{D}\mathbf{Q}^T) = \mathbf{Q}\mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{D}) \quad \forall\mathbf{Q}. \tag{17}$$

Also the second law of thermodynamics [Eq.(3)] requires that

$$\mathbf{f}(\theta, O.P., -\nabla\theta, \mathbf{D}) = -\mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{D}). \tag{18}$$

Since the velocity strain tensor $\mathbf{D}$ is a real, symmetric tensor, it has three real eigenvalues. The three eigenvalues can be distinct, identical, or two of them can be identical. In the present work, we focus on the case that the three eigenvalues are distinct. Similar results may be obtained for the other two cases.

Theorem 4. $\nabla\theta, \mathbf{D}\nabla\theta, \mathbf{D}^2\nabla\theta$ *are linearly independent if three eigenvalues of* $\mathbf{D}$ *are distinct.*

Proof Let μ_k and $\mathbf{f}_k$ $(k = 1, 2, 3)$ to be the eigenvalues and eigenvectors of $\mathbf{D}$. $\mathbf{D}$ may be represented, in its spectral form, as

$$\mathbf{D} = \sum_{k=1}^{3} \mu_k \mathbf{f}_k \otimes \mathbf{f}_k. \tag{19}$$

The linear independence of $\mathbf{f}_k (k = 1, 2, 3)$ allows us to write $\nabla\theta$ as

$$\nabla\theta = (\nabla\theta)_j \mathbf{f}_j \tag{20}$$

in which $(\nabla\theta)_j = \nabla\theta \cdot \mathbf{f}_j$.

Suppose that $\nabla\theta, \mathbf{D}\nabla\theta$ and $\mathbf{D}^2\nabla\theta$ are linearly dependent for all $\mathbf{D}$ and $\nabla\theta$, there are α, β and γ which are not all zero, such that

$$\alpha\nabla\theta + \beta\mathbf{D}\nabla\theta + \gamma\mathbf{D}^2\nabla\theta = \mathbf{0}. \tag{21}$$

Substituting (19) and (20) into (21) yields

$$\sum_{k=1}^{3}(\alpha + \beta\mu_k + \gamma\mu_k^2)(\nabla\theta)_k\mathbf{f}_k = 0, \tag{22}$$

which implies, as $\mathbf{f}_k$ $(k = 1, 2, 3)$ are linearly independent,

$$(\alpha + \beta\mu_k + \gamma\mu_k^2)(\nabla\theta)_k = 0, \quad (k = 1, 2, 3). \tag{23}$$

For arbitrary $\nabla\theta$, $(\nabla\theta)_k$ need not be zero, so

$$\alpha + \beta\mu_k + \gamma\mu_k^2 = 0, \quad (k = 1, 2, 3) \tag{24}$$

that requires that $\alpha = \beta = \gamma = 0$ for distinct μ_k, contrary to the hypothesis. Theorem 4 has, thus, been proved.

Applying Theorem 4 to the SGS flux vector, we have

$$\begin{aligned}\mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{D}) = {}& \phi_0(\theta, O.P., \nabla\theta, \mathbf{D})\nabla\theta + \phi_1(\theta, O.P., \nabla\theta, \mathbf{D})\mathbf{D}\nabla\theta \\ & + \phi_2(\theta, O.P., \nabla\theta, \mathbf{D})\mathbf{D}^2\nabla\theta,\end{aligned} \tag{25}$$

and

$$\begin{aligned}\mathbf{f}(\theta, O.P., -\nabla\theta, \mathbf{D}) = {}& -\phi_0(\theta, O.P., -\nabla\theta, \mathbf{D})\nabla\theta \\ & -\phi_1(\theta, O.P., -\nabla\theta, \mathbf{D})\mathbf{D}\nabla\theta - \phi_2(\theta, O.P., -\nabla\theta, \mathbf{D})\mathbf{D}^2\nabla\theta.\end{aligned} \tag{26}$$

Substituting (25) and (26) into (18) leads to

$$\begin{aligned}&[\phi_0(\theta, O.P., \nabla\theta, \mathbf{D}) - \phi_0(\theta, O.P., -\nabla\theta, \mathbf{D})]\nabla\theta \\ &+[\phi_1(\theta, O.P., \nabla\theta, \mathbf{D}) - \phi_1(\theta, O.P., -\nabla\theta, \mathbf{D})]\mathbf{D}\nabla\theta \\ &+[\phi_2(\theta, O.P., \nabla\theta, \mathbf{D}) - \phi_2(\theta, O.P., -\nabla\theta, \mathbf{D})]\mathbf{D}^2\nabla\theta = 0\end{aligned} \tag{27}$$

which implies, since $\nabla\theta, \mathbf{D}\nabla\theta$ and $\mathbf{D}^2\nabla\theta$ are linearly independent,

$$\phi_i(\theta, O.P., \nabla\theta, \mathbf{D}) = \phi_i(\theta, O.P., -\nabla\theta, \mathbf{D}), \quad (i = 0, 1, 2). \tag{28}$$

To satisfy this requirement, take

$$\phi_i(\theta, O.P., \nabla\theta, \mathbf{D}) = \psi_i(\theta, O.P., \nabla\theta \otimes \nabla\theta, \mathbf{D}), \quad (i = 0, 1, 2). \tag{29}$$

Then (25) and (29) result in

$$\mathbf{f}(\theta, O.P., \mathbf{Q}\nabla\theta, \mathbf{Q}\mathbf{D}\mathbf{Q}^T) = \mathbf{Q}(\hat{\psi}_0\nabla\theta + \hat{\psi}_1\mathbf{D}\nabla\theta + \hat{\psi}_2\mathbf{D}^2\nabla\theta) \tag{30}$$

in which,

$$\hat{\psi}_i = \psi_i(\theta, O.P., \mathbf{Q}\nabla\theta \otimes \mathbf{Q}\nabla\theta, \mathbf{QDQ}^T),$$

and

$$\mathbf{Qf}(\theta, O.P., \nabla\theta, \mathbf{D}) = \mathbf{Q}(\psi_0\nabla\theta + \psi_1\mathbf{D}\nabla\theta + \psi_2\mathbf{D}^2\nabla\theta). \tag{31}$$

By making use of (30) and (31), (17) yields

$$(\hat{\psi}_0 - \psi_0)\nabla\theta + (\hat{\psi}_1 - \psi_1)\mathbf{D}\nabla\theta + (\hat{\psi}_2 - \psi_2)\mathbf{D}^2\nabla\theta = \mathbf{0} \tag{32}$$

that implies, by Theorem 4,

$$\psi_i(\theta, O.P., \mathbf{Q}\nabla\theta \otimes \mathbf{Q}\nabla\theta, \mathbf{QDQ}^T) = \psi_i(\theta, O.P., \nabla\theta \otimes \nabla\theta, \mathbf{D}) \quad \forall\mathbf{Q}. \tag{33}$$

Theorem 5. *Suppose*

$$\psi(\theta, O.P., \mathbf{Qb} \otimes \mathbf{Qb}, \mathbf{QBQ}^T) = \psi(\theta, O.P., \mathbf{b} \otimes \mathbf{b}, \mathbf{B}), \quad \forall\mathbf{b} \textit{ and } \mathbf{B},$$

then

$$\psi(\theta, O.P., \mathbf{a} \otimes \mathbf{a}, \mathbf{A}) = \psi(\theta, O.P., \mathbf{b} \otimes \mathbf{b}, \mathbf{B})$$

whenever $J_k(\mathbf{a}, \mathbf{A}) = J_k(\mathbf{b}, \mathbf{B}) \quad (k = 1, 2, \cdots, 6)$. *Here*

$$\begin{array}{lll} J_1(\mathbf{a}, \mathbf{A}) = tr\mathbf{A}, & J_2(\mathbf{a}, \mathbf{A}) = \frac{1}{2}[(tr\mathbf{A})^2 - tr(\mathbf{A}^2)], & J_3(\mathbf{a}, \mathbf{A}) = det\mathbf{A}, \\ J_4(\mathbf{a}, \mathbf{A}) = \mathbf{a} \cdot \mathbf{Aa}, & J_5(\mathbf{a}, \mathbf{A}) = \mathbf{a} \cdot \mathbf{A}^2\mathbf{a}, & J_6(\mathbf{a}, \mathbf{A}) = \mid \mathbf{a} \mid, \end{array}$$

a *and* **b** *are two arbitrary vectors,* **A** *and* **B** *are two arbitrary symmetric tensors.*

Proof Since $J_k(\mathbf{a}, \mathbf{A}) = J_k(\mathbf{b}, \mathbf{B})$ $(k = 1, 2, 3)$, tensors **A** and **B** have same eigenvalues. Let μ_k be their eigenvalues, **A** and **B** may be written as,

$$\mathbf{A} = \sum_{k=1}^{3} \mu_k \mathbf{e}_k \otimes \mathbf{e}_k, \quad \mathbf{B} = \sum_{k=1}^{3} \mu_k \mathbf{f}_k \otimes \mathbf{f}_k$$

where $\mathbf{e}_k$ and $\mathbf{f}_k$ $(k = 1, 2, 3)$ are eigenvectors of **A** and **B**, respectively. Define

$$\mathbf{Q} = \mathbf{e}_k \otimes \mathbf{f}_k$$

that is a rotation tensor, and

$$\mathbf{e}_i = \mathbf{Qf}_i, \quad \mathbf{A} = \mathbf{QBQ}^T, \quad \mathbf{A}^2 = \mathbf{QB}^2\mathbf{Q}^T, \quad (i = 1, 2, 3). \tag{34}$$

By applying $J_k(\mathbf{a}, \mathbf{A}) = J_k(\mathbf{b}, \mathbf{B})$ $(k = 4, 5, 6)$, we have

$$\begin{array}{ll} \sum_{k=1}^{3} (\mathbf{b} \cdot \mathbf{f}_k)^2 = \sum_{k=1}^{3} (\mathbf{Q}^T\mathbf{a} \cdot \mathbf{f}_k)^2, & \sum_{k=1}^{3} \mu_k (\mathbf{b} \cdot \mathbf{f}_k)^2 = \sum_{k=1}^{3} \mu_k (\mathbf{Q}^T\mathbf{a} \cdot \mathbf{f}_k)^2, \\ \sum_{k=1}^{3} \mu_k^2 (\mathbf{b} \cdot \mathbf{f}_k)^2 = \sum_{k=1}^{3} \mu_k^2 (\mathbf{Q}^T\mathbf{a} \cdot \mathbf{f}_k)^2. & \end{array} \tag{35}$$

This implies, for the distinct μ_k $(k = 1, 2, 3)$,

$$(\mathbf{Q}^T \mathbf{a} \mp \mathbf{b}) \cdot \mathbf{f}_k = 0, \quad (k = 1, 2, 3). \tag{36}$$

Note that $\mathbf{f}_k$ $(k = 1, 2, 3)$ are linearly independent, then $\mathbf{a} = \pm \mathbf{Qb}$, $\mathbf{a} \otimes \mathbf{a} = \mathbf{Qb} \otimes \mathbf{Qb}$. By hypothesis,

$$\psi(\theta, O.P., \mathbf{b} \otimes \mathbf{b}, \mathbf{B}) = \psi(\theta, O.P., \mathbf{Qb} \otimes \mathbf{Qb}, \mathbf{QBQ}^T) = \psi(\theta, O.P., \mathbf{a} \otimes \mathbf{a}, \mathbf{A})$$

in which $\mathbf{A} = \mathbf{QBQ}^T$ [(34)] and $\mathbf{a} \otimes \mathbf{a} = \mathbf{Qb} \otimes \mathbf{Qb}$ are used. Therefore,

$$\psi(\theta, O.P., \mathbf{b} \otimes \mathbf{b}, \mathbf{B}) = \psi[\theta, O.P., J_k(\mathbf{b}, \mathbf{B})], \quad (k = 1, 2, \cdots, 6) \tag{37}$$

if

$$\psi(\theta, O.P., \mathbf{Qb} \otimes \mathbf{Qb}, \mathbf{QBQ}^T) = \psi(\theta, O.P., \mathbf{b} \otimes \mathbf{b}, \mathbf{B}), \quad \forall \mathbf{b} \text{ and } \mathbf{B}. \tag{38}$$

The converse is also true since $J_k(\mathbf{Qb}, \mathbf{QBQ}^T) = J_k(\mathbf{b}, \mathbf{B})$ $(k = 1, 2, \cdots, 6)$.

Theorem 6. *The necessary condition for the constitutive process (1) to satisfy requirements (2) and (3) is*

$$\mathbf{q} = \mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{D}) = (\phi_0 \mathbf{1} + \phi_1 \mathbf{D} + \phi_2 \mathbf{D}^2)\nabla\theta$$

where

$$\phi_i = \phi_i[\theta, O.P., J_k(\nabla\theta, \mathbf{D})], \quad (i = 0, 1, 2;\ k = 1, 2, \cdots, 6).$$

Proof Applying Theorem 5 to (33) yields

$$\psi_i(\theta, O.P., \nabla\theta \otimes \nabla\theta, \mathbf{D}) = \psi_i[\theta, O.P., J_k(\nabla\theta, \mathbf{D})]. \tag{39}$$

This, with (25) and (29), leads to

$$\mathbf{q} = \mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{D}) = (\phi_0 \mathbf{1} + \phi_1 \mathbf{D} + \phi_2 \mathbf{D}^2)\nabla\theta \tag{40}$$

where

$$\phi_i = \phi_i[\theta, O.P., J_k(\nabla\theta, \mathbf{D})], \quad (i = 0, 1, 2;\ k = 1, 2, \cdots, 6).$$

If the three eigenvalues of $\mathbf{D}$ are not distinct, we can still obtain (40) with $\phi_1 = \phi_2 = 0$ (for the case of three identical eigenvalues) or $\phi_2 = 0$ (for the case of two identical eigenvalues) by the similar method. Therefore, (40) is valid for all cases.

2.2. SUFFICIENCY OF (40) FOR REQUIREMENTS (2) AND (3)

Suppose (40) holds, then

$$\begin{aligned}&\mathbf{f}(\theta^*, O.P.^*, (\nabla\theta^*)^*, \mathbf{v}^*, \mathbf{L}^*) = \{\phi_0(\theta^*, O.P.^*, J_k((\nabla\theta^*)^*, \mathbf{D}^*))\mathbf{1}\\&+\phi_1(\theta^*, O.P.^*, J_k((\nabla\theta^*)^*, \mathbf{D}^*))\mathbf{D}^* + \phi_2(\theta^*, O.P.^*, J_k((\nabla\theta^*)^*, \mathbf{D}^*))\mathbf{D}^{*2}\}\\&(\nabla\theta^*)^* = \{\phi_0(\theta, O.P., J_k(\mathbf{Q}\nabla\theta, \mathbf{QDQ}^T))\mathbf{Q1Q}^T + \phi_1(\theta, O.P., J_k(\mathbf{Q}\nabla\theta,\\&\mathbf{QDQ}^T))\mathbf{QDQ}^T + \phi_2(\theta, O.P., J_k(\mathbf{Q}\nabla\theta, \mathbf{QDQ}^T))\mathbf{QD}^2\mathbf{Q}^T\}\mathbf{Q}\nabla\theta\\&= \mathbf{Q}\{\phi_0(\theta, O.P., J_k(\mathbf{Q}\nabla\theta, \mathbf{QDQ}^T))\mathbf{1} + \phi_1(\theta, O.P., J_k(\mathbf{Q}\nabla\theta, \mathbf{QDQ}^T))\\&\mathbf{D} + \phi_2(\theta, O.P., J_k(\mathbf{Q}\nabla\theta, \mathbf{QDQ}^T))\mathbf{D}^2\}\mathbf{Q}^T\mathbf{Q}\nabla\theta\\&= \mathbf{Qf}(\theta, O.P., \nabla\theta, \mathbf{v}, \mathbf{L}) = \mathbf{q}^*, \quad (k = 1, 2, \cdots, 6)\end{aligned} \tag{41}$$

in which Eq.(5), $\mathbf{D}^* = \mathbf{QDQ}^T$ and $J_k(\mathbf{Q}\nabla\theta, \mathbf{QDQ}^T) = J_k(\nabla\theta, \mathbf{D})$ $(k = 1, 2, \cdots, 6)$ are used.

Also, if (40) holds,

$$\begin{aligned}&\mathbf{f}(\theta, O.P., -\nabla\theta, \mathbf{v}, \mathbf{L}) = \{\phi_0(\theta, O.P., J_k(-\nabla\theta, \mathbf{D}))\mathbf{1}\\&+\phi_1(\theta, O.P., J_k(-\nabla\theta, \mathbf{D}))\mathbf{D} + \phi_2(\theta, O.P., J_k(-\nabla\theta, \mathbf{D}))\mathbf{D}^2\}(-\nabla\theta)\\&= -\{\phi_0(\theta, O.P., J_k(\nabla\theta, \mathbf{D}))\mathbf{1} + \phi_1(\theta, O.P., J_k(\nabla\theta, \mathbf{D}))\mathbf{D}\\&+\phi_2(\theta, O.P., J_k(\nabla\theta, \mathbf{D}))\mathbf{D}^2\}(\nabla\theta) = -\mathbf{f}(\theta, O.P., \nabla\theta, \mathbf{v}, \mathbf{L}), (k = 1, 2, \cdots, 6)\end{aligned} \tag{42}$$

in which $J_k(-\nabla\theta, \mathbf{D}) = J_k(\nabla\theta, \mathbf{D})$ $(k = 1, 2, \cdots, 6)$ are used. Equations (41) and (42) establish the sufficiency of (40) for (2) and (3).

2.3. PROPERTIES OF ϕ_I $(I = 0, 1, 2)$ AND BOTH NECESSARY AND SUFFICIENT CONDITIONS FOR INEQUALITY (4)

Both necessity and sufficiency of (40) for Eqs.(2) and (3) are established in §2.1 and §2.2. Here we analyze some fundamental properties of ϕ_i $(i = 0, 1, 2)$, and develop both necessary and sufficient conditions for inequality (4).

Rewrite Eq.(40) as

$$\mathbf{q} = -\mathbf{K}\nabla\theta, \tag{43}$$

with

$$\mathbf{K} = -(\phi_0\mathbf{1} + \phi_1\mathbf{D} + \phi_2\mathbf{D}^2) = \varphi_0\mathbf{1} + \varphi_1\mathbf{D} + \varphi_2\mathbf{D}^2. \tag{44}$$

Here $\mathbf{1}$ is a unit (identity) tensor, and

$$\varphi_i = -\phi_i \quad (i = 0, 1, 2). \tag{45}$$

$\mathbf{K}$ has two fundamental properties: (1) it is a real-valued tensor on the ground of practical transport processes, and (2) it is a symmetric tensor due to the symmetry of velocity strain tensor $\mathbf{D}$.

Let λ_j and f_j $(j = 1,2,3)$ be the three eigenvalues of **D** and **K**, respectively. Since **K** is related to **D** through Eq.(44),

$$f_j = \varphi_0 + \varphi_1 \lambda_j + \varphi_2 \lambda_j^2, \quad (j = 1,2,3). \tag{46}$$

Because **D** and **K** are real-valued symmetric tensors, λ_j and f_j $(j = 1,2,3)$ must be real-valued, i.e.,

$$\overline{f}_j = f_j, \quad (j = 1,2,3), \tag{47}$$

$$\overline{\lambda}_j = \lambda_j, \quad (j = 1,2,3). \tag{48}$$

By Eq.(46),

$$\overline{f}_j = \overline{\varphi}_0 + \overline{\varphi}_1 \overline{\lambda}_j + \overline{\varphi}_2 \overline{\lambda}_j^2, \quad (j = 1,2,3). \tag{49}$$

By making use of Eqs.(47) and (48), Eq.(49) leads to

$$f_j = \overline{\psi}_0 + \overline{\varphi}_1 \lambda_j + \overline{\varphi}_2 \lambda_j^2, \quad (j = 1,2,3). \tag{50}$$

This, with Eq.(46), yields

$$(\varphi_0 - \overline{\varphi}_0) + (\varphi_1 - \overline{\varphi}_1)\lambda_j + (\varphi_2 - \overline{\varphi}_2)\lambda_j^2 = 0, \quad (j = 1,2,3), \quad \forall \lambda_j \in R \tag{51}$$

which indicates that

$$\varphi_i = \overline{\varphi}_i \quad (i = 0,1,2). \tag{52}$$

Therefore, φ_i $(i = 0,1,2)$ must be real-valued.

Substituting Eq.(43) into inequality (4) yields

$$\nabla\theta \cdot \mathbf{K}\nabla\theta \geq 0, \qquad \forall \nabla\theta, \tag{53}$$

which implies that **K** is positive semi-definite. Note also that **K** is, in practice, an invertible tensor, it must be positive definite. The same conclusion may be obtained by noting that the equal sign in (4) is only for reversible processes and transport processes are irreversible.

The necessary and sufficient condition for a symmetric tensor to be positive definite is that all of its eigenvalues are positive definite. Both necessary and sufficient condition for inequality (4) is, thus,

$$\varphi_0 + \varphi_1 \lambda_j + \varphi_2 \lambda_j^2 > 0, \quad (j = 1,2,3), \quad \forall \lambda_j \in R. \tag{54}$$

Two necessary conditions of (54) can be easily obtained by considering cases of $\lambda_j = 0$ and $\mid \lambda_j \mid \to \infty$, respectively, as

$$\varphi_0 > 0, \tag{55}$$

$$\varphi_2 > 0. \tag{56}$$

Dividing (54) by φ_0, we can rearrange (54) into an alternative form

$$(1 + \frac{\varphi_1 \lambda_j}{2\varphi_0})^2 + (\frac{\varphi_2}{\varphi_0} - \frac{\varphi_1^2}{4\varphi_0^2})\lambda_j^2 > 0 \quad \forall \lambda_j \in R. \tag{57}$$

This yields another necessary condition, by setting $\lambda_j = -2\varphi_0/\varphi_1$,

$$\varphi_1^2 - 4\varphi_0\varphi_2 < 0. \tag{58}$$

Conversely, it is easy to show that (55), (56) and (58) are also the sufficient conditions of (54).

The detailed expressions of φ_0, φ_1 and φ_2 are material-dependent and need to be determined through experiments. Once they are determined, Eq. (43) can serve as the SGS flux model that is properly invariant and satisfies the second law of thermodynamics.

3. Concluding Remarks

For a class of turbulence flows for which the SGS flux vector can be described by Eq.(1), both necessary and sufficient conditions are derived in a systematic, rigorous way for the invariance, the PMFI and the second law of thermodynamics. This leads to a general model (43) with three real-valued functions φ_i ($i = 0, 1, 2$) satisfying (55) (56) and (58). Any specific model satisfying (43), (55), (56) and (58) is properly invariant and satisfies the second law of thermodynamics while the model violating these conditions is not. The work is believed to be important both for developing the specific, physics-preserving models and for clarifying some confusion in the literature by noting that the previous works employ an intuitive approach with the focus on only obtaining the sufficient condition.

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